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Title: AI Enhanced Discretizations for High-Fidelity Physics Simulations

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AI Enhanced Discretizations for High-Fidelity Physics Simulations

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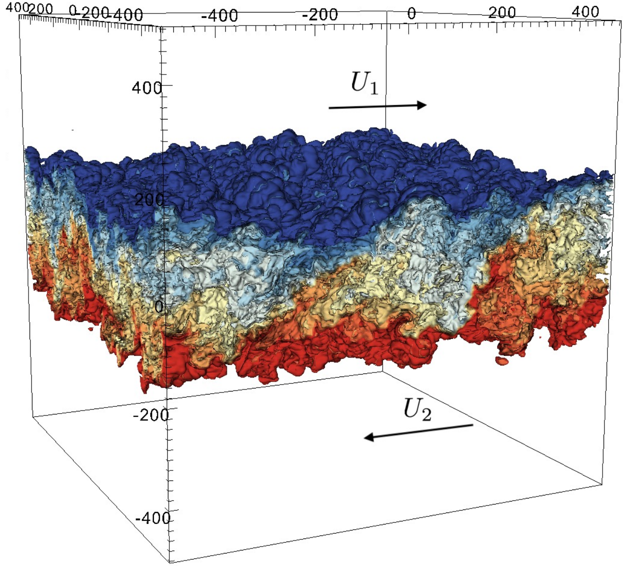
CCS-2

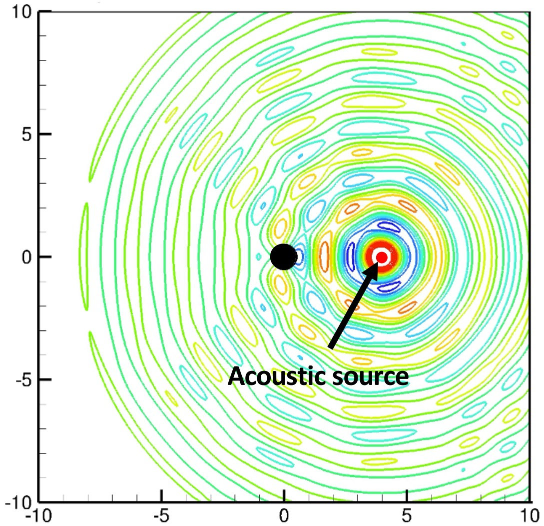
Introduction

- Non-dissipative schemes are preferred for high-fidelity turbulent flow and aeroacoustics simulations
- Practical applications need stable boundary closures that ensure stability without adding artificial (numerical) dissipation

Turbulent mixing layer



Acoustic scatter

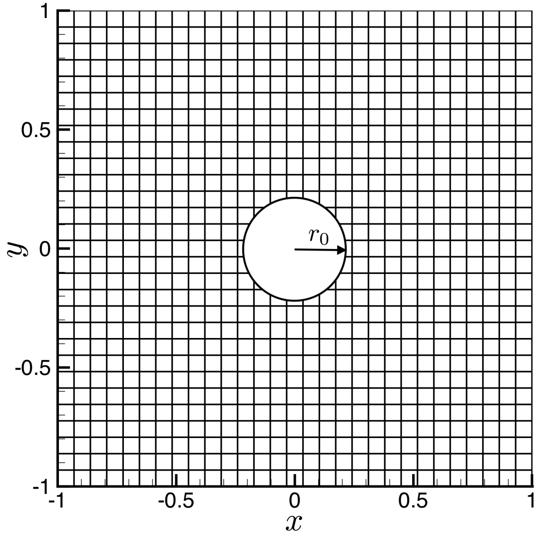


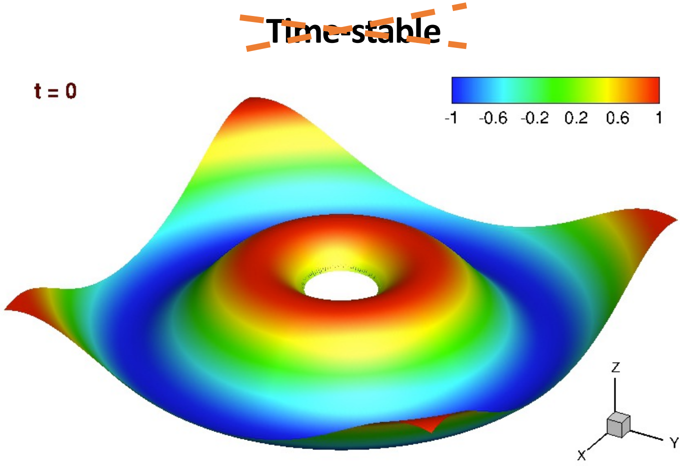
Boundary instabilities with non-dissipative schemes

Time stability. A method is **time-stable** if for homogenous boundary data and no source terms, there is a unique solution $\mathbf{u}(t)$ satisfying

$$\|\mathbf{u}\|_{\Delta x} \leq K \|\mathbf{f}\|_{\Delta x}, \qquad \text{or} \qquad \frac{d}{dt}\|\mathbf{u}\|^2_{\Delta x} \leq 0,$$

where K is independent of Δx, **f** and t. **f** denotes the initial data.





Sufficient conditions for time stability

- For a semidiscrete approximation

$$\frac{d\mathbf{v}}{dt} = M\mathbf{v} + \mathbf{b}$$

$$\mathbf{v}(0) = \mathbf{f}(x),$$

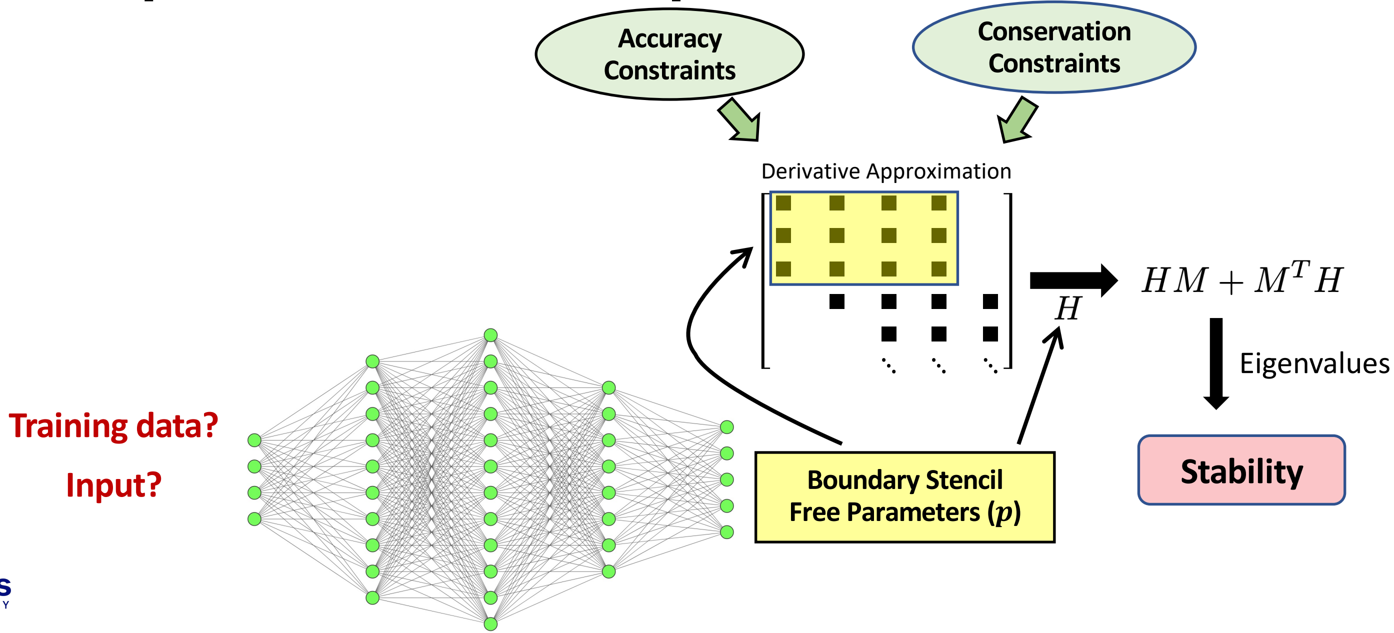
$$M = \text{system matrix} \qquad \mathbf{b} = \text{boundary data}$$

- Sufficient conditions for time-stability:
  - All eigenvalues of M have non-positive real part and the geometric multiplicity of every eigenvalue with zero real part is equal to its algebraic multiplicity
  - There exists a real symmetric positive definite matrix H such that $\mathbf{x}^T HM\mathbf{x} \leq 0$ for all $\mathbf{x} \Rightarrow M^T H + HM$ is negative semidefinite

Derivation of time-stable boundary stencils for centered schemes

$$D = \frac{1}{\Delta x}\begin{bmatrix} d_{10} & \cdots & \cdots & \cdots & \cdots & d_{1\beta} & & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & & & \\ d_{\kappa 0} & \cdots & \cdots & \cdots & \cdots & d_{\kappa\beta} & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & -c_w & \cdots & -c_1 & 0 & c_1 & \cdots & c_w \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

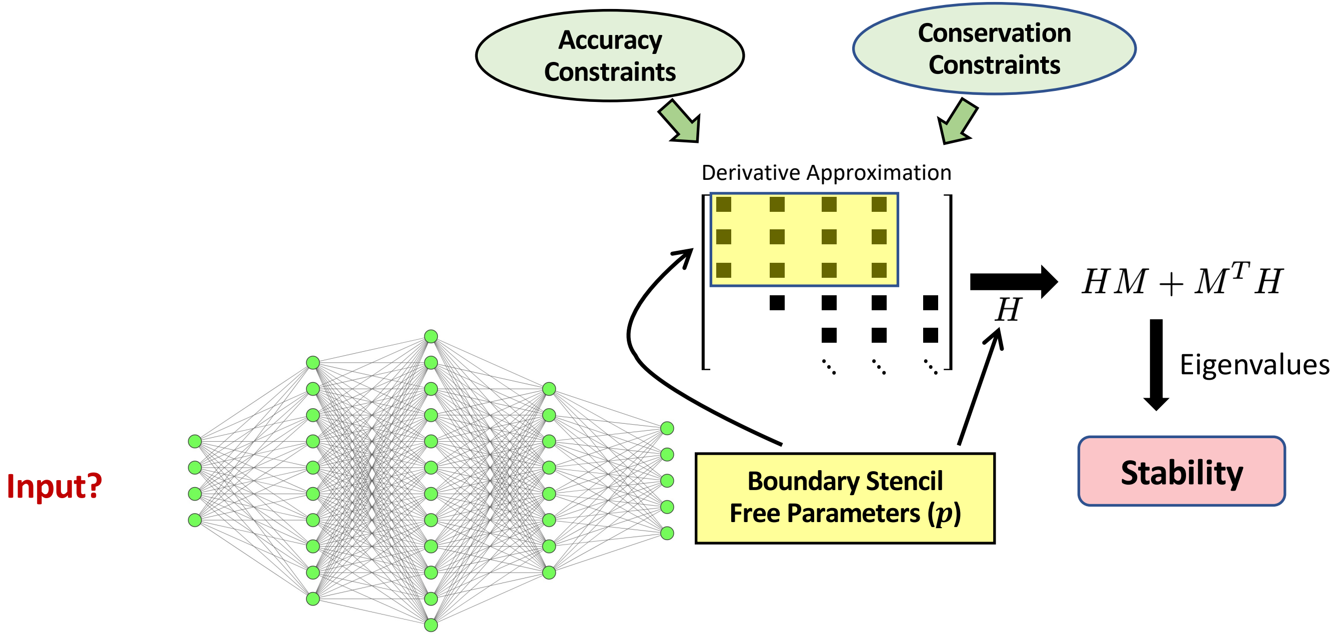
$$H = \Delta x \begin{bmatrix} h_{11} & \cdots & \cdots & h_{1\kappa} & & \\ \vdots & \ddots & \ddots & \vdots & & \\ \vdots & \ddots & \ddots & \vdots & & \\ h_{\kappa 1} & \cdots & \cdots & h_{\kappa\kappa} & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix}$$



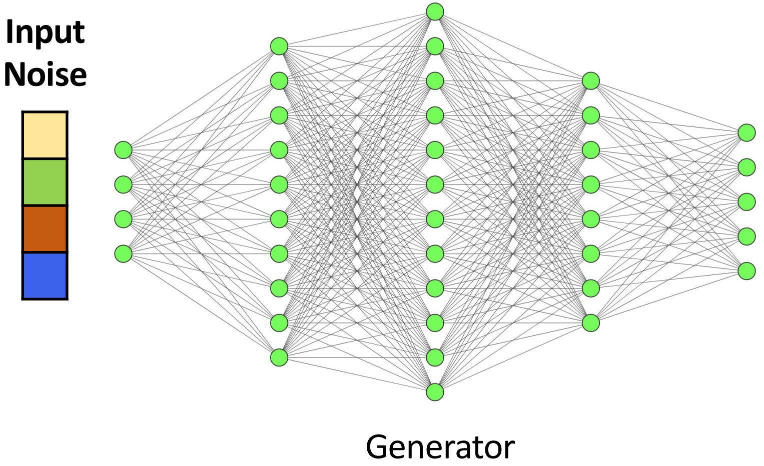
Derivation of time-stable boundary stencils for centered schemes

Cost Function

$$J = \mathrm{loss}(\mathbf{\Lambda}_{\mathcal{L}}^{+}, \sigma_{\mathcal{L}}\mathbf{I}_{\mathcal{L}}^{+}) + \mathrm{loss}(\mathbf{\Lambda}_{H}^{-}, \sigma_{H}\mathbf{I}_{H}^{-}) = \sum_{i=0}^{n-1}\left(\Lambda_{\mathcal{L},i}^{+} - \sigma_{\mathcal{L}} I_{\mathcal{L},i}^{+}\right)^2 + \sum_{i=0}^{n-1}\left(\Lambda_{H,i}^{-} - \sigma_{H} I_{H,i}^{-}\right)^2$$

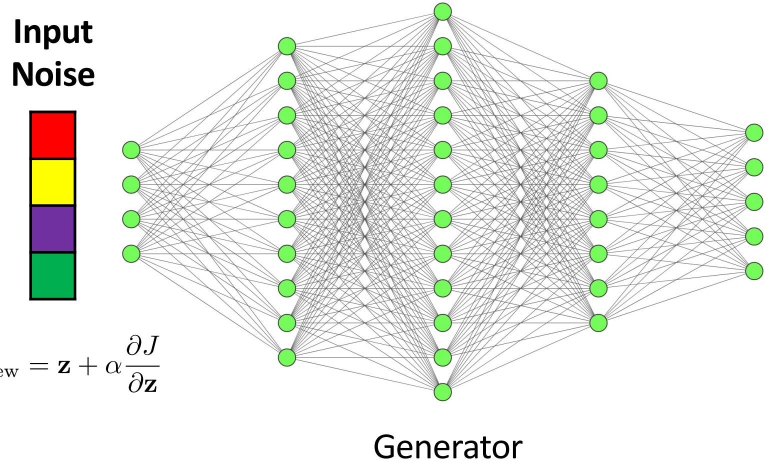


Controllable generation in image synthesis



Shen et al. (2020)

Controllable generation in image synthesis

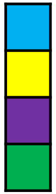


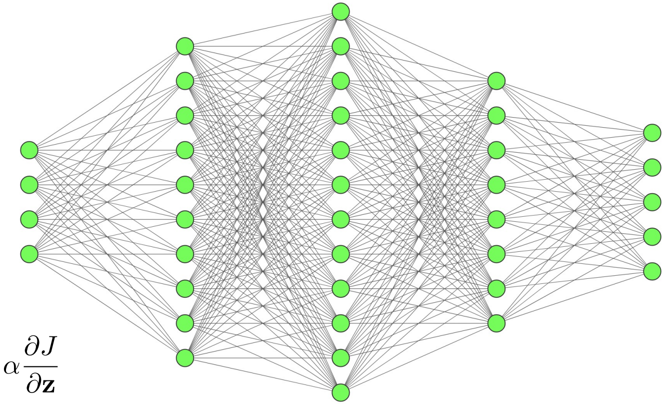
$$\mathbf{z}_{\text{new}} = \mathbf{z} + \alpha \frac{\partial J}{\partial \mathbf{z}}$$

Shen et al. (2020)

Controllable generation in image synthesis

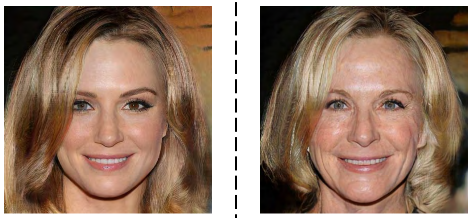
Input Noise





Generator

$$\mathbf{z}_{\text{new}} = \mathbf{z} + \alpha \frac{\partial J}{\partial \mathbf{z}}$$

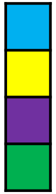


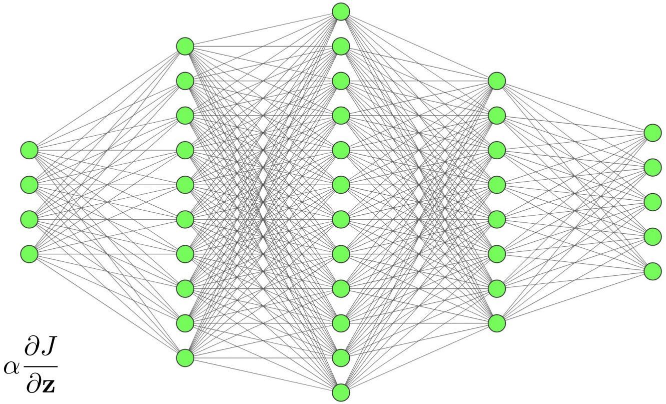
Original Age

Shen et al. (2020)

Controllable generation in image synthesis

Input Noise





$$\mathbf{z}_{\text{new}} = \mathbf{z} + \alpha \frac{\partial J}{\partial \mathbf{z}}$$

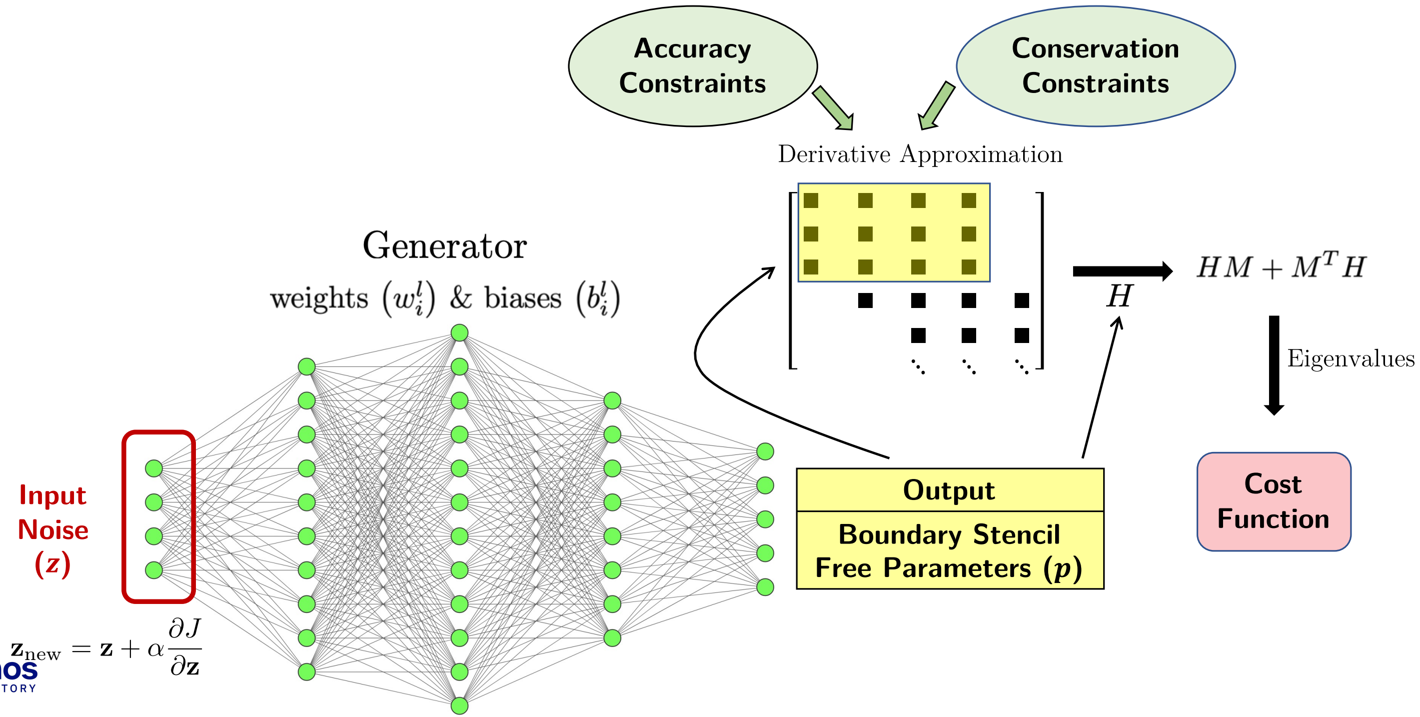
Generator

Original | Age | Eyeglasses | Gender | Pose

Shen et al. (2020)

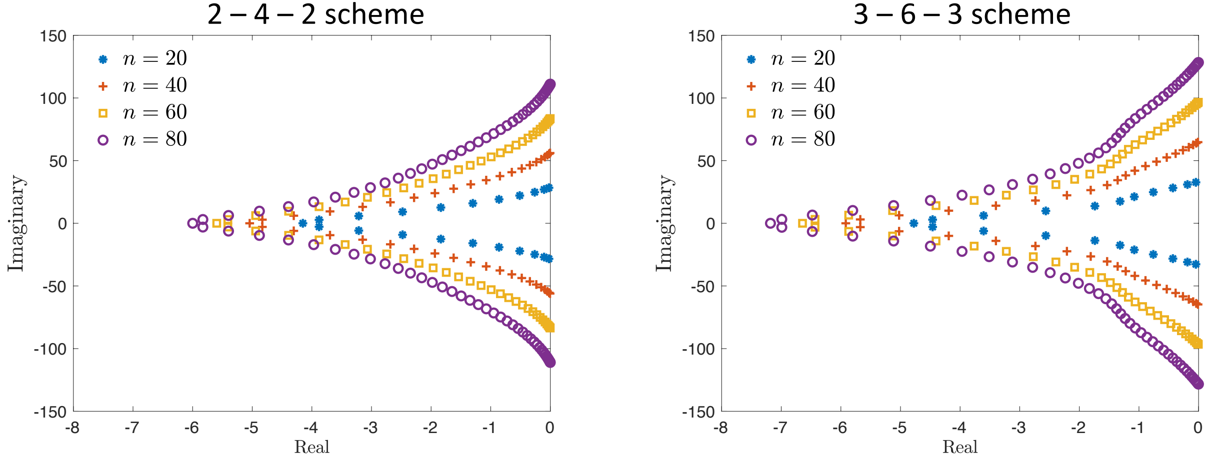
Controllable generation of boundary stencils

- Step 1: Coarse-grained search ➡ Fix the weights and biases
- Step 2: Finer modifications to the noise vector for time stability



Numerical results: Scalar hyperbolic problem

Eigenvalue spectrum from the derived schemes



Convergence rate

n	2 – 4 – 2 scheme				3 – 6 – 3 scheme			
	$\log_{10} \|\|\varepsilon\|\|_2$	Rate	$\log_{10} \|\|\varepsilon\|\|_\infty$	Rate	$\log_{10} \|\|\varepsilon\|\|_2$	Rate	$\log_{10} \|\|\varepsilon\|\|_\infty$	Rate
20	-1.973422		-1.703554		-2.279161		-1.948476	
40	-2.916809	3.134	-2.574815	2.894	-3.449783	3.889	-3.196234	4.145
80	-3.835924	3.053	-3.486709	3.029	-4.631867	3.927	-4.366281	3.887
160	-4.745814	3.023	-4.384746	2.983	-5.826623	3.969	-5.557024	3.956
320	-5.651926	3.010	-5.282615	2.983	-7.026841	3.987	-6.756342	3.984
640	-6.556365	3.004	-6.197129	3.038	-8.229245	3.994	-7.958516	3.994

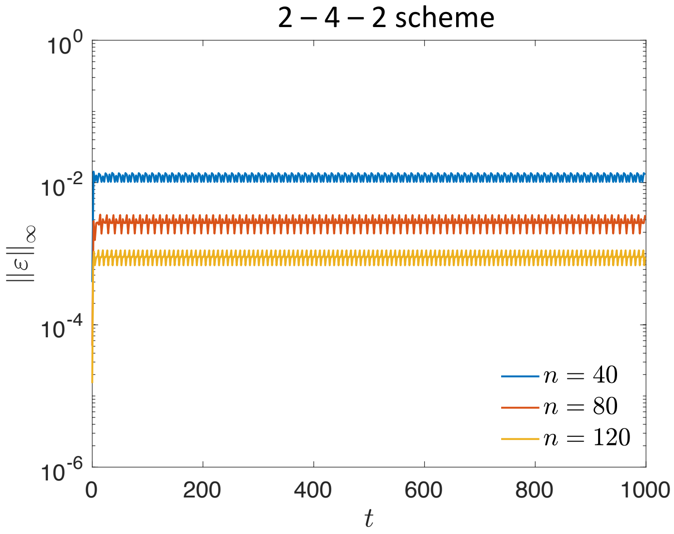
Numerical results: Inviscid Burgers' equation

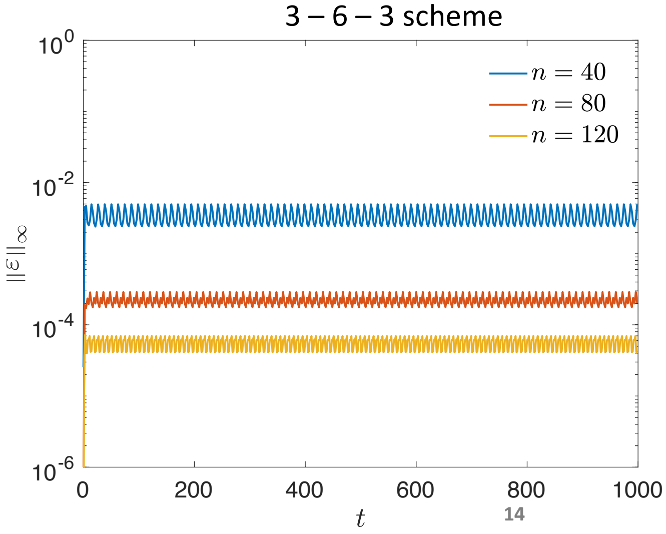
$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}\left(\frac{U^2}{2}\right) = f_U. \qquad 0 \le x \le 1,\ t \ge 0,$$

$$U(x,t) = \sin 2\pi (x-t) + C,$$

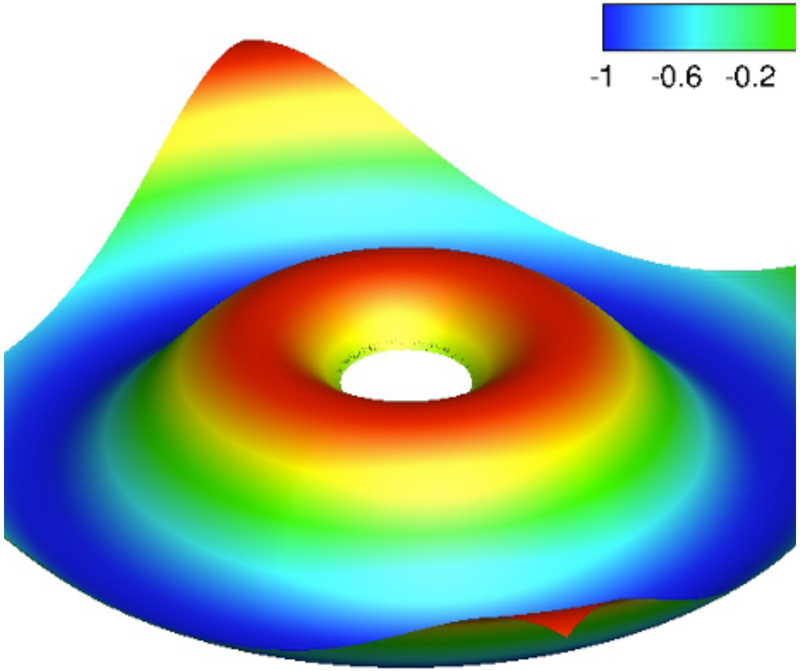
$$f_U(x,t) = \pi \sin 4\pi (x-t).$$

Stability





AI Enhanced Discretizations for High-Fidelity Physics Simulations



Time stable simulation of varying coefficient scalar hyperbolic equation

Project Description:

Combine theoretical analysis with deep learning to design efficient numerical discretizations for direct numerical simulations of fluid flow.

Project Outcomes:
Developed a controllable generation approach using deep NN to derive time-stable, high-order numerical schemes for high-fidelity physics simulations.

PI: Peter Brady
Total Project Budget: 60k
ISTI Focus Area: Data Science and AI Infrastructure / Simulation

END